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 31-33 33-34 33-35 35-36 35-40 36-37 36-38

exact/norm bonds :
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exact bonds :
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G1:H,CH3,n-Bu,i-Bu,s-Bu,t-Bu,Ph,Cb,Ak

G2:cb,Ak

G3: Cy, Ak, CH3, n-Bu, i-Bu, s-Bu, t-Bu

Match level :

1:CLASS 2:CLASS 3:CLASS 4:CLASS 5:CLASS 6:CLASS 7:CLASS 8:CLASS 9:CLASS 10:CLASS  
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USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.  
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.  
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FILE COVERS 1907 - 25 Sep 2003 VOL 139 ISS 13  
FILE LAST UPDATED: 24 Sep 2003 (20030924/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

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18916699 PY<1999  
L4 0 L3 AND PY<1999

=> T3 and py<2000  
19719652 PY<2000  
L5 1 L3 AND PY<2000

=> d bib

L5 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2003 ACS on STN  
AN 1999:795834 CAPLUS  
DN 132:36034  
TI Preparation of peptide inhibitors of hepatitis C virus NS3 protease  
IN Matassa, Victor; Narjes, Frank; Koehler, Konrad; Ontoria, Jesus; Poma, Marco; Marchetti, Antonella  
PA Istituto Di Ricerche Di Biologia Molecolare P Angeletti S.p.A., Italy  
SO PCT Int. Appl., 121 pp.  
CODEN: PIXXD2  
DT Patent  
LA English  
FAN.CNT 1

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CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG  
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AU 9942798 A1 19991230 AU 1999-42798 19990609 <--  
AU 754773 B2 20021121  
EP 1084137 A1 20010321 EP 1999-955475 19990609  
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PRAI GB 1998-12523 A 19980610  
WO 1999-GB1824 W 19990609  
RE.CNT 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD  
ALL CITATIONS AVAILABLE IN THE RE FORMAT

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L9 4 L8

=> l9 and py<2000  
19719652 PY<2000  
L10 1 L9 AND PY<2000

=> d bib 1

L10 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2003 ACS on STN  
 AN 1999:795834 CAPLUS  
 DN 132:36034  
 TI Preparation of peptide inhibitors of hepatitis C virus NS3 protease  
 IN Matassa, Victor; Narjes, Frank; Koehler, Konrad; Ontoria, Jesus; Poma, Marco; Marchetti, Antonella  
 PA Istituto Di Ricerche Di Biologia Molecolare P Angeletti S.p.A., Italy  
 SO PCT Int. Appl., 121 pp.  
 CODEN: PIXXD2  
 DT Patent  
 LA English  
 FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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	EP 1084137	A1	20010321	EP 1999-955475	19990609
PRAI	GB 1998-12523	A	19980610		
	WO 1999-GB1824	W	19990609		

RE.CNT 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD  
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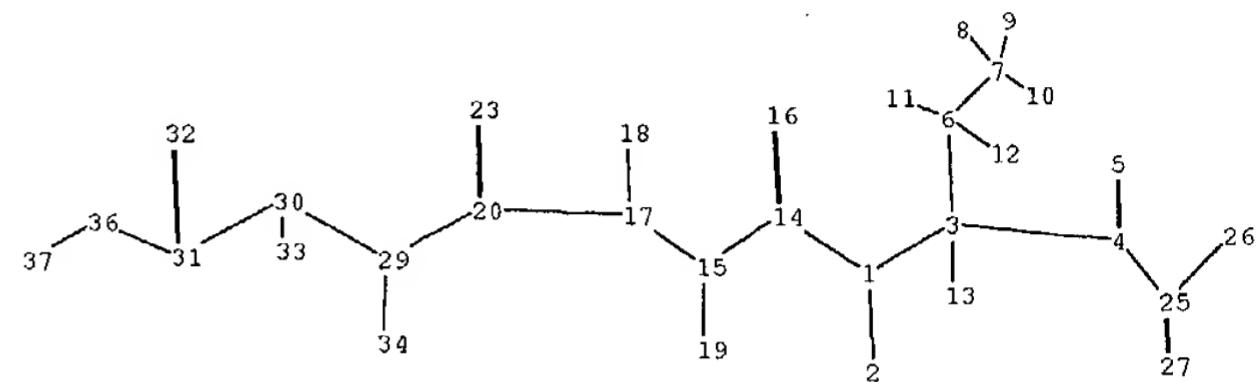
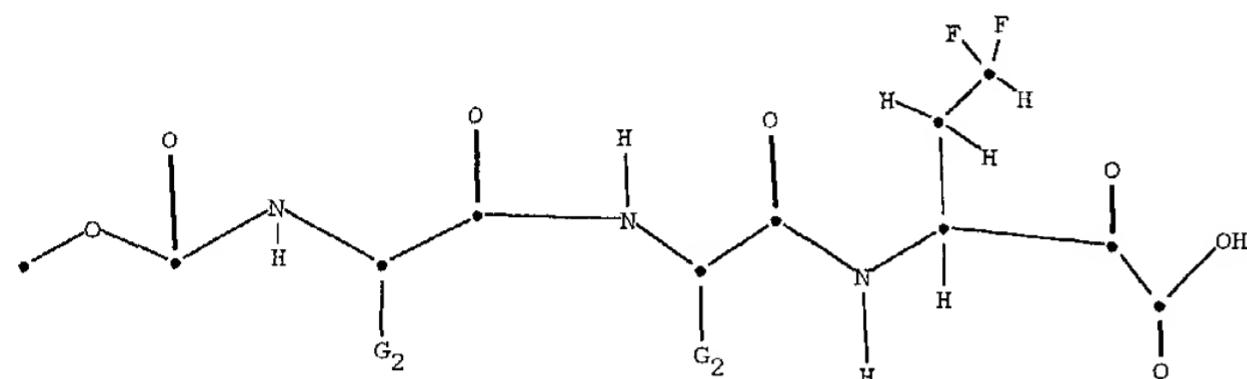
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L9 ANSWER 2 OF 4 CAPLUS COPYRIGHT 2003 ACS on STN  
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 DN 137:149812  
 TI A designed P1 cysteine mimetic for covalent and non-covalent inhibitors of HCV NS3 protease  
 AU Narjes, Frank; Koehler, Konrad F.; Koch, Uwe; Gerlach, Benjamin; Colarusso, Stefania; Steinkuhler, Christian; Brunetti, Mirko; Altamura, Sergio; De Francesco, Raffaele; Matassa, Victor G.  
 CS Department of Chemistry, MRL Rome, IRBM, Rome, Pomezia, 00040, Italy  
 SO Bioorganic & Medicinal Chemistry Letters (2002), 12(4), 701-704  
 CODEN: BMCLE8; ISSN: 0960-894X  
 PB Elsevier Science Ltd.  
 DT Journal  
 LA English  
 RE.CNT 27 THERE ARE 27 CITED REFERENCES AVAILABLE FOR THIS RECORD  
ALL CITATIONS AVAILABLE IN THE RE FORMAT

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L9 ANSWER 3 OF 4 CAPLUS COPYRIGHT 2003 ACS on STN  
 AN 2000:68910 CAPLUS  
 DN 132:245829  
 TI .alpha.-Ketoacids Are Potent Slow Binding Inhibitors of the Hepatitis C virus NS3 Protease  
 AU Narjes, Frank; Brunetti, Mirko; Colarusso, Stefania; Gerlach, Benjamin; Koch, Uwe; Biasiol, Gabriella; Fattori, Daniela; De Francesco, Raffaele; Matassa, Victor G.; Steinkuehler, Christian  
 CS Departments of Biochemistry Medicinal Chemistry and Computational Chemistry, Istituto di Ricerche di Biologia Molecolare (IRBM) P. Angeletti, Pomezia, 00040, Italy  
 SO Biochemistry (2000), 39(7), 1849-1861  
 CODEN: BICHAW; ISSN: 0006-2960



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  30 31 32 33 34 36 37

chain bonds :
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  15-17 15-19 17-18 17-20 20-23 20-29 25-26 25-27 29-30 29-34 30-31 30-33 31-32
  31-36 36-37

exact/norm bonds :
  1-3  1-14  4-5  14-16  15-17  15-19  17-20  20-23  29-30  29-34  30-31  31-32  31-36
  36-37

exact bonds :
  1-2  3-13  3-6  3-4  4-25  6-7  6-11  6-12  7-8  7-9  7-10  14-15  17-18  20-29  30-33

normalized bonds :
  25-26 25-27

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G1:H,CH3,n-Bu,i-Bu,s-Bu,t-Bu,Ph,Cb,Ak

G2:cb,Ak

G3: Cy, Ak, CH3, n-Bu, i-Bu, s-Bu, t-Bu

G4:Hy, H

Match level :

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PB American Chemical Society

DT Journal

LA English

RE.CNT 58 THERE ARE 58 CITED REFERENCES AVAILABLE FOR THIS RECORD  
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L18 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2003 ACS on STN  
AN 1999:795834 CAPLUS  
DN 132:36034  
TI Preparation of peptide inhibitors of hepatitis C virus NS3 protease  
IN Matassa, Victor; Narjes, Frank; Koehler, Konrad; Ontoria, Jesus; Poma, Marco; Marchetti, Antonella  
PA Istituto Di Ricerche Di Biologia Molecolare P Angeletti S.p.A., Italy  
SO PCT Int. Appl., 121 pp.  
CODEN: PIXXD2  
DT Patent  
LA English  
FAN.CNT 1  
PATENT NO. KIND DATE APPLICATION NO. DATE  
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PI WO 9964442 A1 19991216 WO 1999-GB1824 19990609  
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JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK,  
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CA 2330247 AA 19991216 CA 1999-2330247 19990609  
AU 9942798 A1 19991230 AU 1999-42798 19990609  
AU 754773 B2 20021121  
EP 1084137 A1 20010321 EP 1999-955475 19990609  
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE  
PRAI GB 1998-12523 A 19980610  
WO 1999-GB1824 W 19990609  
RE.CNT 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD  
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L24 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2003 ACS on STN  
AN 1999:795834 CAPLUS  
DN 132:36034  
TI Preparation of peptide inhibitors of hepatitis C virus NS3 protease  
IN Matassa, Victor; Narjes, Frank; Koehler, Konrad; Ontoria, Jesus; Poma, Marco; Marchetti, Antonella  
PA Istituto Di Ricerche Di Biologia Molecolare P Angeletti S.p.A., Italy  
SO PCT Int. Appl., 121 pp.

CODEN: PIXXD2  
DT Patent  
LA English

FAN.CNT 1

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RE.CNT 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD  
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L4 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2003 ACS on STN  
AN 1999:795834 CAPLUS  
DN 132:36034  
TI Preparation of peptide inhibitors of hepatitis C virus NS3 protease  
IN Matassa, Victor; Narjes, Frank; Koehler, Konrad; Ontoria, Jesus; Poma,  
Marco; Marchetti, Antonella  
PA Istituto Di Ricerche Di Biologia Molecolare P Angeletti s.p.A., Italy  
SO PCT Int. Appl., 121 pp.  
CODEN: PIXXD2

DT Patent

LA English

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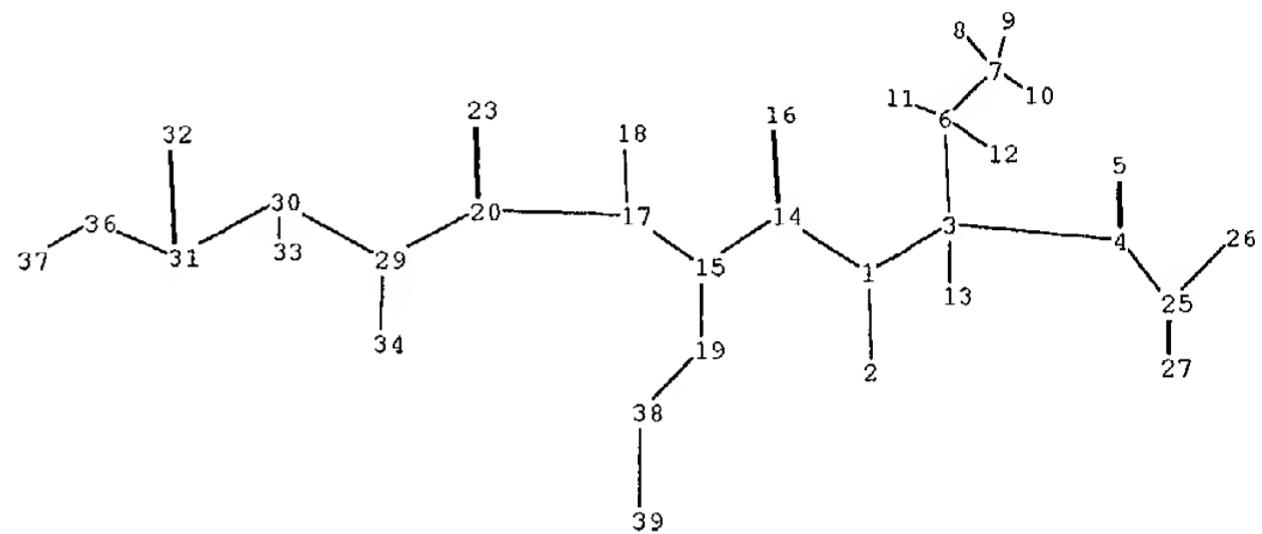
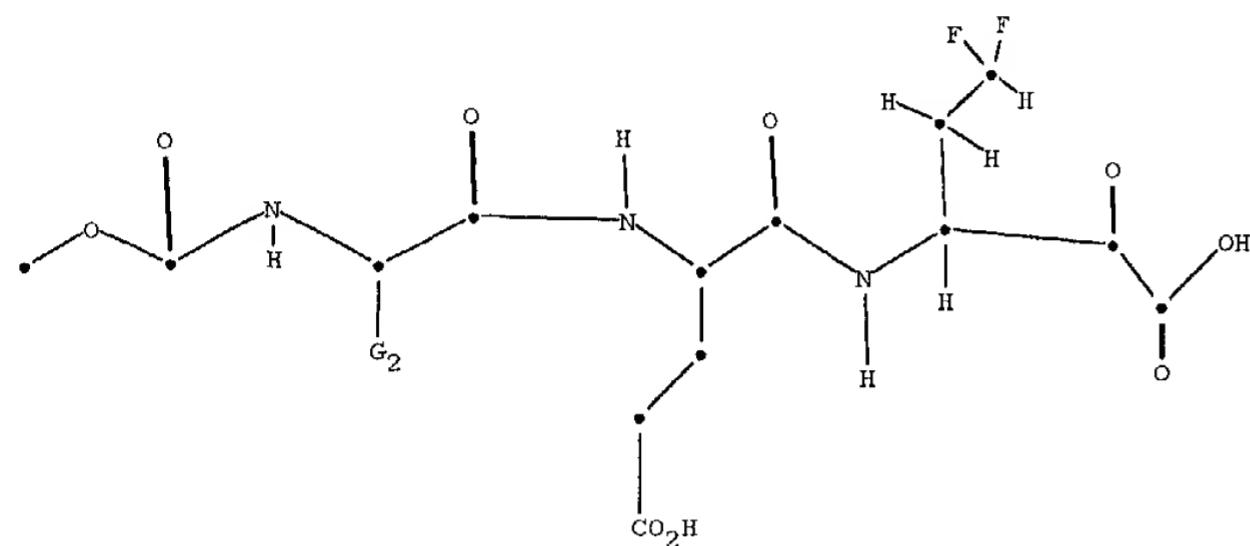
RE.CNT 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD  
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 15-17 15-19 17-18 17-20 19-38 20-23 20-29 25-26 25-27 29-30 29-34 30-31 30-33
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exact/norm bonds :
 1-3 1-14 4-5 14-16 15-17 17-20 20-23 29-30 29-34 30-31 31-32 31-36 36-37

exact bonds :
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normalized bonds :
 25-26 25-27

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G1:H,CH3,n-Bu,i-Bu,s-Bu,t-Bu,Ph,Cb,Ak

G2:cb,Ak

G3: Cy, Ak, CH3, n-Bu, i-Bu, s-Bu, t-Bu

G4:Hy, H

Match Level :

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DN 132:36034  
TI Preparation of peptide inhibitors of hepatitis C virus NS3 protease  
IN Matassa, Victor; Narjes, Frank; Koehler, Konrad; Ontoria, Jesus; Poma, Marco; Marchetti, Antonella  
PA Istituto Di Ricerche Di Biologia Molecolare P Angeletti S.p.A., Italy  
SO PCT Int. Appl., 121 pp.  
CODEN: PIXXD2

DT Patent

LA English

FAN.CNT 1

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	EP 1084137	A1	20010321	EP 1999-955475	19990609
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PRAI	GB 1998-12523	A	19980610		
	WO 1999-GB1824	W	19990609		

RE.CNT 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD  
ALL CITATIONS AVAILABLE IN THE RE FORMAT

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3 ANSWERS

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L3 5 L2

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18916701 PY<1999

L4 0 L3 AND PY<1999

=> 13 and py<2000  
19719654 PY<2000

L5 1 L3 AND PY<2000

=> d bib

L5 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2003 ACS on STN  
AN 1999:795834 CAPLUS  
DN 132:36034  
TI Preparation of peptide inhibitors of hepatitis C virus NS3 protease  
IN Matassa, Victor; Narjes, Frank; Koehler, Konrad; Ontoria, Jesus; Poma, Marco; Marchetti, Antonella  
PA Istituto Di Ricerche Di Biologia Molecolare P Angeletti S.p.A., Italy  
SO PCT Int. Appl., 121 pp.  
CODEN: PIXXD2

DT Patent  
LA English

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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	AU 9942798	A1	19991230	AU 1999-42798	19990609 <--
	AU 754773	B2	20021121		
	EP 1084137	A1	20010321	EP 1999-955475	19990609
PRAI	GB 1998-12523	A	19980610	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE	
	WO 1999-GB1824	W	19990609		

RE.CNT 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD  
ALL CITATIONS AVAILABLE IN THE RE FORMAT

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Uploading italianhcvi.str

L6 STRUCTURE UPLOADED

=> 16 sss full  
\*\*\* REGISTRY INITIATED \*\*\*  
Substance data SEARCH and crossover from CAS REGISTRY in progress...  
Use DISPLAY HITSTR (or FHITSTR) to directly view retrieved structures.

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SEARCH TIME: 00.00.01

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L8 6 L7

=> 18 and py<2000  
19719654 PY<2000  
L9 1 L8 AND PY<2000

=> d bib

L9 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2003 ACS on STN  
AN 1999:795834 CAPLUS  
DN 132:36034  
TI Preparation of peptide inhibitors of hepatitis C virus NS3 protease  
IN Matassa, Victor; Narjes, Frank; Koehler, Konrad; Ontoria, Jesus; Poma, Marco; Marchetti, Antonella  
PA Istituto Di Ricerche Di Biologia Molecolare P Angeletti S.p.A., Italy  
SO PCT Int. Appl., 121 pp.  
CODEN: PIXXD2

DT Patent  
LA English  
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 9964442	A1	19991216	WO 1999-GB1824	19990609 <--
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	AU 9942798	A1	19991230	AU 1999-42798	19990609 <--
	AU 754773	B2	20021121		
	EP 1084137	A1	20010321	EP 1999-955475	19990609
PRAI	GB 1998-12523	A	19980610	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE	
	WO 1999-GB1824	W	19990609		

RE.CNT 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD  
ALL CITATIONS AVAILABLE IN THE RE FORMAT

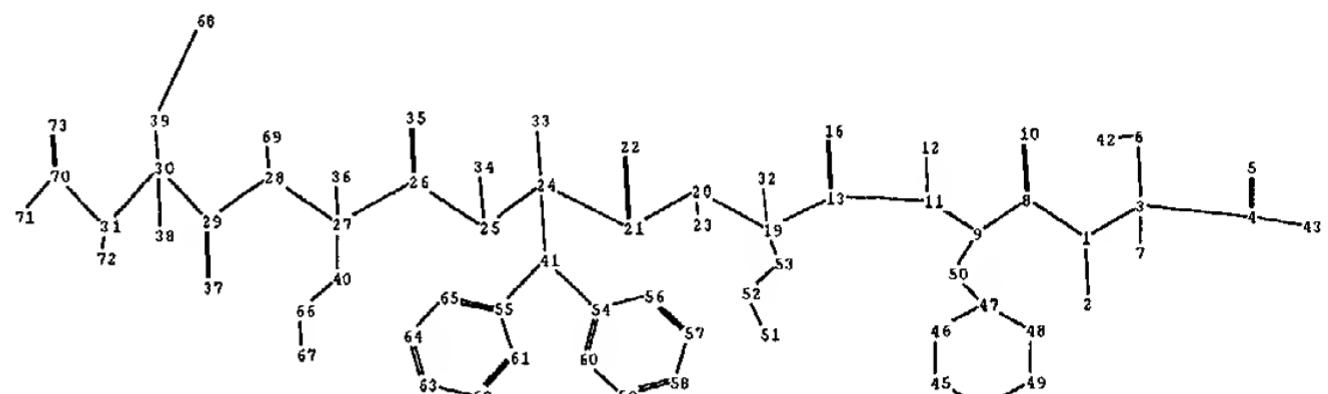
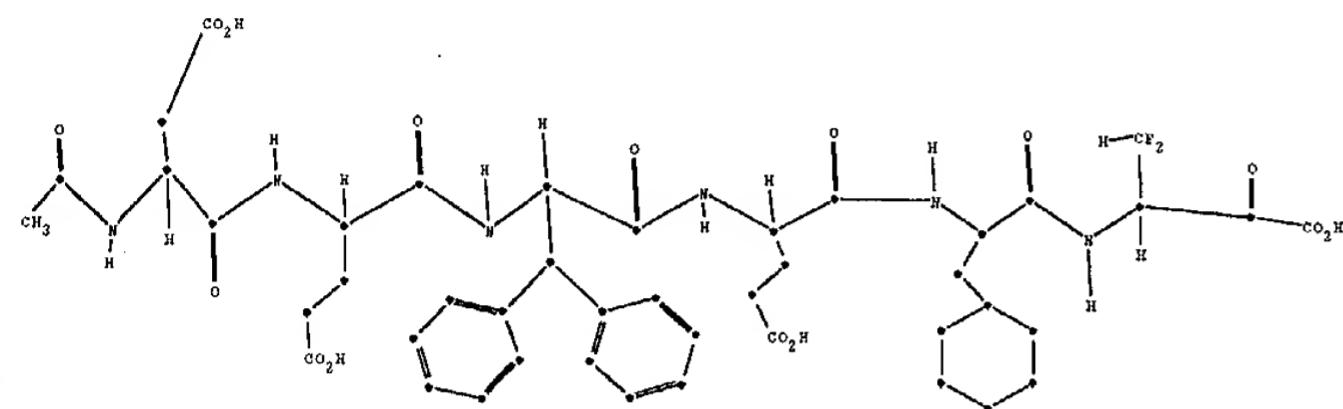
=> d 13 ab 1-5

L3 ANSWER 1 OF 5 CAPLUS COPYRIGHT 2003 ACS on STN  
AB N-Terminal truncation of the hexapeptide ketoacid MeCO-Asp-Glu-NHCH(CHPh2)CO-Glu-NHCH(CH2c-C6H11)CONHCH(CH2CHF2)CO2H (all-L stereochem.) (c-C6H11= cyclohexyl) gave rise to potent tripeptide inhibitors of the hepatitis C virus NS3 protease/NS4A cofactor complex. Optimization of these tripeptides led to ketoacid BOC-NHCH(c-C5H9)CO-Leu-NHCH(CH2CHF2)COCO2H (all-L stereochem.) (BOC = tert-butoxycarbonyl, c-C5H9 = cyclopentyl) with an IC50 of 0.38 .mu.M. The SAR of these tripeptides is discussed in the light of the recently published crystal structures of a ternary tripeptide/NS3/NS4A complexes.

L3 ANSWER 2 OF 5 CAPLUS COPYRIGHT 2003 ACS on STN  
AB The difluoromethyl group was designed by computational chem. methods as a mimetic of the canonical P1 cysteine thiol for inhibitors of the hepatitis C virus NS3 protease. This modification led to the development of competitive, non-covalent inhibitor AcAspGlu-NHCH(CHPh2)CO-Glu-NHCH(CH2C6H11)CONHCH(CH2CHF2)R (I, R = CHO) Ki 30 nM and reversible covalent inhibitors (I, R = CO2H) Ki 0.5 nM; and (I, R = COCO2H) Ki\* 10 pM.

L3 ANSWER 3 OF 5 CAPLUS COPYRIGHT 2003 ACS on STN  
AB A serine protease domain contained within the viral NS3 protein is a key player in the maturational processing of the hepatitis C virus polyprotein and a prime target for the development of antiviral drugs. In the present work, we describe a dansylated hexapeptide inhibitor of this enzyme. Active site occupancy by this compd. could be monitored following fluorescence resonance energy transfer between the dansyl fluorophore and protein tryptophan residues and could be used to (1) unambiguously assess active site binding of NS3 protease inhibitors, (2) directly det. equil. and pre-steady-state parameters of enzyme-inhibitor complex formation, and (3) dissect, using site-directed mutagenesis, the contribution of single residues of NS3 to inhibitor binding in direct binding assays. The assay was also used to characterize the inhibition of the NS3 protease by its cleavage products. We show that enzyme-product inhibitor complex formation depends on the presence of an NS4A cofactor peptide. Equil. and pre-steady-state data support an ordered mechanism of ternary (enzyme-inhibitor-cofactor) complex formation, requiring cofactor complexation prior to inhibitor binding.

L3 ANSWER 4 OF 5 CAPLUS COPYRIGHT 2003 ACS on STN  
AB The replication of the hepatitis C virus (HCV), an important human pathogen, crucially depends on the proteolytic maturation of a large viral polyprotein precursor. The viral nonstructural protein 3 (NS3) harbors a serine protease domain that plays a pivotal role in this process, being responsible for four out of the five cleavage events that occur in the nonstructural region of the HCV polyprotein. We here show that hexapeptide, tetrapeptide, and tripeptide .alpha.-ketoacids are potent, slow binding inhibitors of this enzyme. Their mechanism of inhibition



**chain nodes :**  
 1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23 24 25 26 27 28 29  
 30 31 32 33 34 35 36 37 38 39 40 41 42 43 44 45 46 47 48 49 50 51 52 53 54 55 56 57 58 59 60 61 62 63 64 65  
 70 71 72 73

**ring nodes :**  
 44 45 46 47 48 49 54 55 56 57 58 59 60 61 62 63 64 65

**chain bonds :**  
 1-2 1-3 1-8 3-7 3-6 3-4 4-5 4-43 6-42 8-9 8-10 9-11 9-50 11-12 11-13 13-16  
 13-19 19-20 19-32 19-53 20-21 20-23 21-22 21-24 24-25 24-33 24-41 25-26 25-34  
 26-27 26-35 27-28 27-36 27-40 28-29 28-69 29-30 29-37 30-31 30-38 30-39 31-70  
 31-72 39-68 40-66 41-54 41-55 47-50 51-52 52-53 66-67 70-71 70-73

**ring bonds :**  
 44-45 44-49 45-46 46-47 47-48 48-49 54-60 54-56 55-65 55-61 56-57 57-58 58-59  
 59-60 61-62 62-63 63-64 64-65

**exact/norm bonds :**  
 1-3 1-8 4-5 8-10 9-11 11-13 13-16 19-20 20-21 21-22 24-25 25-26 26-35 27-28  
 28-29 29-37 30-31 31-70 44-45 44-49 45-46 46-47 47-48 48-49 70-73

**exact bonds :**  
 1-2 3-7 3-6 3-4 4-43 6-42 8-9 9-50 11-12 13-19 19-32 19-53 20-23 21-24  
 24-33 24-41 25-34 26-27 27-36 27-40 28-69 29-30 30-38 30-39 31-72 39-68 40-66  
 41-54 41-55 47-50 51-52 52-53 66-67 70-71

**normalized bonds :**  
 54-60 54-56 55-65 55-61 56-57 57-58 58-59 59-60 61-62 62-63 63-64 64-65

G1:H,CH3,n-Bu,i-Bu,s-Bu,t-Bu,Ph,Cb,Ak

G2:Cb,Ak

G3:Cy,Ak,CH3,n-Bu,i-Bu,s-Bu,t-Bu

G4:Hy,H

Match level :

1:CLASS 2:CLASS 3:CLASS 4:CLASS 5:CLASS 6:CLASS 7:CLASS 8:CLASS 9:CLASS 10:CLASS  
11:CLASS 12:CLASS 13:CLASS 16:CLASS 19:CLASS 20:CLASS 21:CLASS 22:CLASS 23:CLASS  
24:CLASS 25:CLASS 26:CLASS 27:CLASS 28:CLASS 29:CLASS 30:CLASS 31:CLASS 32:CLASS  
33:CLASS 34:CLASS 35:CLASS 36:CLASS 37:CLASS 38:CLASS 39:CLASS 40:CLASS 41:CLASS  
42:CLASS 43:CLASS 44:Atom 45:Atom 46:Atom 47:Atom 48:Atom 49:Atom 50:CLASS  
51:CLASS 52:CLASS 53:CLASS 54:Atom 55:Atom 56:Atom 57:Atom 58:Atom 59:Atom  
60:Atom 61:Atom 62:Atom 63:Atom 64:Atom 65:Atom 66:CLASS 67:CLASS 68:CLASS  
69:CLASS 70:CLASS 71:CLASS 72:CLASS 73:CLASS

29/09/2003 14:50 Print selected from italyanhcvinii.trn

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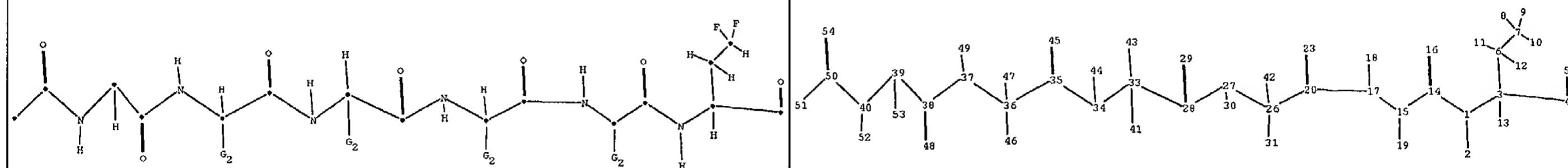
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100.0% PROCESSED 15 ITERATIONS 0 ANSWERS  
SEARCH TIME: 00.00.01

L6 0 SEA SSS FUL L4



chain nodes :

1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	23	26	27	28	29
30	31	33	34	35	36	37	38	39	40	41	42	43	44	45	46	47	48	49	50	51	52			
53	54																							

chain bonds :

1-2	1-3	1-14	3-13	3-6	3-4	4-5	6-7	6-11	6-12	7-8	7-9	7-10	14-15	14-16	15-17	
15-19	17-18	17-20	20-23	20-26	26-27	26-31	26-42	27-28	27-30	28-29	28-33	33-34				
33-41	33-43	34-35	34-44	35-36	35-45	36-37	36-46	36-47	37-38	37-49	38-39	38-48				
39-40	39-53	40-50	40-52	50-51	50-54											

exact/norm bonds :

1-3	1-14	4-5	14-16	15-17	15-19	17-20	20-23	26-27	26-31	27-28	28-29	33-34
33-41	34-35	35-45	36-37	36-46	37-38	38-48	39-40	40-50	50-54			

exact bonds :

1-2	3-13	3-6	3-4	6-7	6-11	6-12	7-8	7-9	7-10	14-15	17-18	20-26	26-42	27-30	
28-33	33-43	34-44	35-36	36-47	37-49	38-39	39-53	40-52	50-51						

G1:H,CH3,n-Bu,i-Bu,s-Bu,t-Bu,Ph,Cb,Ak

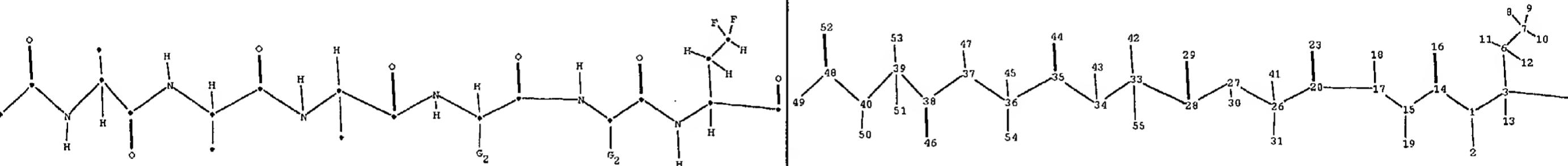
G2:Cb,Ak

G3:Cy,Ak,CH3,n-Bu,i-Bu,s-Bu,t-Bu

G4:Hy,H

Match level :

1:CLASS	2:CLASS	3:CLASS	4:CLASS	5:CLASS	6:CLASS	7:CLASS	8:CLASS	9:CLASS	10:CLASS
11:CLASS	12:CLASS	13:CLASS	14:CLASS	15:CLASS	16:CLASS	17:CLASS	18:CLASS	19:CLASS	
20:CLASS	23:CLASS	26:CLASS	27:CLASS	28:CLASS	29:CLASS	30:CLASS	31:CLASS	33:CLASS	
34:CLASS	35:CLASS	36:CLASS	37:CLASS	38:CLASS	39:CLASS	40:CLASS	41:CLASS	42:CLASS	
43:CLASS	44:CLASS	45:CLASS	46:CLASS	47:CLASS	48:CLASS	49:CLASS	50:CLASS	51:CLASS	
52:CLASS	53:CLASS	54:CLASS							



## chain nodes :

1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	23	26	27	28	29
30	31	33	34	35	36	37	38	39	40	41	42	43	44	45	46	47	48	49	50	49	50	51	52	
53	54	55																						

## chain bonds :

1-2	1-3	1-14	3-13	3-6	3-4	4-5	6-7	6-11	6-12	7-8	7-9	7-10	14-15	14-16	15-17	
15-19	17-18	17-20	20-23	20-26	26-27	26-31	26-41	27-28	27-30	28-29	28-33	33-34				
33-42	33-55	34-35	34-43	35-36	35-44	36-37	36-45	36-54	37-38	37-47	38-39	38-46				
39-40	39-51	39-53	40-48	40-50	48-49	48-52										

## exact/norm bonds :

1-3	1-14	4-5	14-16	15-17	15-19	17-20	20-23	26-27	26-31	27-28	28-29	33-34
34-35	35-44	36-37	37-38	38-46	39-40	40-48	48-52					

## exact bonds :

1-2	3-13	3-6	3-4	6-7	6-11	6-12	7-8	7-9	7-10	14-15	17-18	20-26	26-41	27-30
28-33	33-42	33-55	34-43	35-36	36-45	36-54	37-47	38-39	39-51	39-53	40-50	48-49		

G1:H,CH3,n-Bu,i-Bu,s-Bu,t-Bu,Ph,Cb,Ak

G2:Cb,Ak

G3:Cy,Ak,CH3,n-Bu,i-Bu,s-Bu,t-Bu

G4:Hy,H

## Match level :

1:CLASS	2:CLASS	3:CLASS	4:CLASS	5:CLASS	6:CLASS	7:CLASS	8:CLASS	9:CLASS	10:CLASS
11:CLASS	12:CLASS	13:CLASS	14:CLASS	15:CLASS	16:CLASS	17:CLASS	18:CLASS	19:CLASS	
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43:CLASS	44:CLASS	45:CLASS	46:CLASS	47:CLASS	48:CLASS	49:CLASS	50:CLASS	51:CLASS	
52:CLASS	53:CLASS	54:CLASS	55:CLASS						

involves the rapid formation of a noncovalent collision complex in a diffusion-limited, electrostatically driven assocn. reaction followed by a slow isomerization step resulting in a very tight complex. pH dependence expts. point to the protonated catalytic His 57 as an important determinant for formation of the collision complex. Ki values of the collision complexes vary between 3 nM and 18.5  $\mu$ M and largely depend on contacts made by the peptide moiety of the inhibitors. Site-directed mutagenesis indicates that Lys 136 selectively participates in stabilization of the tight complex but not of the collision complex. A significant solvent isotope effect on the isomerization rate const. is suggestive of a chem. step being rate limiting for tight complex formation. The potency of these compds. is dominated by their slow dissociation rate consts., leading to complex half-lives of 11-48 h and overall Ki values between 10 pM and 67 nM. The rate consts. describing the formation and the dissociation of the tight complex are relatively independent of the peptide moiety and appear to predominantly reflect the intrinsic chem. reactivity of the ketoacid function.

L3 ANSWER 5 OF 5 CAPLUS COPYRIGHT 2003 ACS on STN  
 AB Fluorinated oligopeptides Y-B-A-X or Y-B-A'-X' [A is an amino acid residue NHCH(CH<sub>2</sub>CHF<sub>2</sub>)(CH<sub>2</sub>)<sub>m</sub>CO and A' is NHCHR<sub>1</sub>(CH<sub>2</sub>)<sub>m</sub>CO (m = 0, 1; R<sub>1</sub> is a fluorine-substituted hydrocarbyl side chain); B is a naturally or non-naturally occurring amino acid residue NHCHR<sub>2</sub>CO (R<sub>2</sub> is a nonpolar or polar but uncharged side chain or is a side chain contg. an acidic functionality); X = CO<sub>2</sub>R<sub>8</sub>, H, OR<sub>8</sub>, CF<sub>3</sub>, CONR<sub>9</sub>R<sub>10</sub>, NHO<sub>2</sub>R<sub>25</sub>, or certain 5-membered heterocyclic groups (R<sub>8</sub>, R<sub>9</sub>, R<sub>10</sub>, R<sub>25</sub> = H, alkyl, alkenyl, aryl, aralkyl); X' = NHO<sub>2</sub>N<sub>25</sub>; Y = Z-F-E-D-C (C is a natural or non-natural amino acid residue having non-polar, polar but uncharged, or acidic side chains; D, E, and F may be absent or represent a natural or non-natural amino acid; Z is absent, H, or R<sub>7</sub>CO which forms an amide, urethane, or urea linkage with the nitrogen atom to which it is attached) or R<sub>13</sub>CO (R<sub>13</sub> is an aliph. or arom. group contg. 1-25 carbon atoms, 0-5 oxygen atoms, 0-3 nitrogen atoms, 0-2 sulfur atoms, and up to 9 other heteroatoms)] were prepd. as inhibitors of hepatitis C virus NS3 protease. Thus, Ac-Asp-Glu-Met-Glu-Glu-NHCH(CH<sub>2</sub>CHF<sub>2</sub>)CO<sub>2</sub>H-(S), prepd. by coupling of (S)-tert-Bu 2-amino-4,4-difluorobutanoate hydrochloride with protected pentapeptide, showed IC<sub>50</sub> for inhibition of NS3 protease.

=> d bib 1-5

L9 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2003 ACS on STN  
 AN 1999:795834 CAPLUS  
 DN 132:36034  
 TI Preparation of peptide inhibitors of hepatitis C virus NS3 protease  
 IN Matassa, Victor; Narjes, Frank; Koehler, Konrad; Ontoria, Jesus; Poma, Marco; Marchetti, Antonella  
 PA Istituto Di Ricerche Di Biologia Molecolare P Angeletti S.p.A., Italy  
 SO PCT Int. Appl., 121 pp.  
 CODEN: PIXXD2

DT Patent

LA English

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 9964442	A1	19991216	WO 1999-GB1824	19990609 <--
	W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM	RW: GH, GM, KE, LS, MW, SD, SL, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG			
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	AU 754773	B2	20021121		
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PRAI	GB 1998-12523	A	19980610	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE	
	WO 1999-GB1824	W	19990609		

RE.CNT 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD  
 ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> d 13 bib 1-5

L3 ANSWER 1 OF 5 CAPLUS COPYRIGHT 2003 ACS on STN  
AN 2002:116982 CAPLUS  
DN 137:47425  
TI Evolution, synthesis and SAR of tripeptide  $\alpha$ -ketoacid inhibitors of the hepatitis C virus NS3/NS4A serine protease  
AU Colarusso, Stefania; Gerlach, Benjamin; Koch, Uwe; Muraglia, Ester; Conte, Immacolata; Stansfield, Ian; Matassa, Victor G.; Narjes, Frank  
CS Department of Chemistry, MRL Rome, IRBM, Rome, Pomezia, 00040, Italy  
SO Bioorganic & Medicinal Chemistry Letters (2002), 12(4), 705-708  
CODEN: BMCLE8; ISSN: 0960-894X  
PB Elsevier Science Ltd.  
DT Journal  
LA English  
OS CASREACT 137:47425  
RE.CNT 15 THERE ARE 15 CITED REFERENCES AVAILABLE FOR THIS RECORD  
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 2 OF 5 CAPLUS COPYRIGHT 2003 ACS on STN  
AN 2002:116981 CAPLUS  
DN 137:149812  
TI A designed P1 cysteine mimetic for covalent and non-covalent inhibitors of HCV NS3 protease  
AU Narjes, Frank; Koehler, Konrad F.; Koch, Uwe; Gerlach, Benjamin; Colarusso, Stefania; Steinkuhler, Christian; Brunetti, Mirko; Altamura, Sergio; De Francesco, Raffaele; Matassa, Victor G.  
CS Department of Chemistry, MRL Rome, IRBM, Rome, Pomezia, 00040, Italy  
SO Bioorganic & Medicinal Chemistry Letters (2002), 12(4), 701-704  
CODEN: BMCLE8; ISSN: 0960-894X  
PB Elsevier Science Ltd.  
DT Journal  
LA English  
RE.CNT 27 THERE ARE 27 CITED REFERENCES AVAILABLE FOR THIS RECORD  
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 3 OF 5 CAPLUS COPYRIGHT 2003 ACS on STN  
AN 2000:352482 CAPLUS  
DN 133:189820  
TI Probing the active site of the hepatitis C virus serine protease by fluorescence resonance energy transfer  
AU Fattori, Daniela; Urbani, Andrea; Brunetti, Mirko; Ingenito, Raffaele; Pessi, Antonello; Prendergast, Kristine; Narjes, Frank; Matassa, Victor G.; De Francesco, Raffaele; Steinkuhler, Christian  
CS Istituto di Ricerche di Biologia Molecolare "P. Angeletti", Rome, 00040, Italy  
SO Journal of Biological Chemistry (2000), 275(20), 15106-15113  
CODEN: JBCHA3; ISSN: 0021-9258  
PB American Society for Biochemistry and Molecular Biology  
DT Journal  
LA English  
RE.CNT 42 THERE ARE 42 CITED REFERENCES AVAILABLE FOR THIS RECORD  
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 4 OF 5 CAPLUS COPYRIGHT 2003 ACS on STN  
AN 2000:68910 CAPLUS  
DN 132:245829  
TI  $\alpha$ -Ketoacids Are Potent Slow Binding Inhibitors of the Hepatitis C Virus NS3 Protease  
AU Narjes, Frank; Brunetti, Mirko; Colarusso, Stefania; Gerlach, Benjamin; Koch, Uwe; Biasiol, Gabriella; Fattori, Daniela; De Francesco, Raffaele; Matassa, Victor G.; Steinkuehler, Christian  
CS Departments of Biochemistry Medicinal Chemistry and Computational Chemistry, Istituto di Ricerche di Biologia Molecolare (IRBM) P. Angeletti, Pomezia, 00040, Italy  
SO Biochemistry (2000), 39(7), 1849-1861  
CODEN: BICHAW; ISSN: 0006-2960  
PB American Chemical Society  
DT Journal  
LA English  
RE.CNT 58 THERE ARE 58 CITED REFERENCES AVAILABLE FOR THIS RECORD  
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 5 OF 5 CAPLUS COPYRIGHT 2003 ACS on STN  
AN 1999:795834 CAPLUS  
DN 132:36034

TI Preparation of peptide inhibitors of hepatitis C virus NS3 protease  
IN Matassa, Victor; Narjes, Frank; Koehler, Konrad; Ontoria, Jesus; Poma, Marco; Marchetti, Antonella  
PA Istituto Di Ricerche Di Biologia Molecolare P Angeletti S.p.A., Italy  
SO PCT Int. Appl., 121 pp.  
CODEN: PIXXD2

DT Patent  
LA English

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 9964442	A1	19991216	WO 1999-GB1824	19990609
	W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM	RW: GH, GM, KE, LS, MW, SD, SL, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG			
	CA 2330247	AA	19991216	CA 1999-2330247	19990609
	AU 9942798	A1	19991230	AU 1999-42798	19990609
	AU 754773	B2	20021121		
	EP 1084137	A1	20010321	EP 1999-955475	19990609
	PRAI GB 1998-12523	A	19980610	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE	
	WO 1999-GB1824	W	19990609		

RE.CNT 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD  
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L1 STRUCTURE UPLOADED

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FULL SCREEN SEARCH COMPLETED - 445 TO ITERATE

100.0% PROCESSED 445 ITERATIONS 24 ANSWERS  
SEARCH TIME: 00.00.01

L2 24 SEA SSS FUL L1

=> l2  
L3 6 l2

=> D bib 1-6

L3 ANSWER 1 OF 6 CAPLUS COPYRIGHT 2003 ACS on STN  
AN 2002:777963 CAPLUS  
DN 137:295254  
TI Preparation of peptide inhibitors of hepatitis C virus NS3 protease  
IN Colarusso, Stefania; Gardelli, Cristina; Gerlach, Benjamin; Harper, Steven; Koch, Uwe; Matassa, Victor Giulio; Muraglia, Ester; Narjes, Frank; Ontoria, Ontoria Jesus Maria; Petrocchi, Alessia; Ponzi, Simona; Stansfield, Ian; Summa, Vincenzo  
PA Istituto di Ricerche di Biologia Molecolare P. Angeletti Spa, Italy; et al.  
SO PCT Int. Appl., 151 pp.  
CODEN: PIXXD2

DT Patent  
LA English

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2002079234	A1	20021010	WO 2002-EP3435	20020326
	W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM	RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR,			

BF, BJ, CF, CG, CL, CM, GA, GN, GQ, GW, ML, MR, NE, N, TD, TG  
PRAI GB 2001-7924 A 20020329

OS MARPAT 137:295254

RE.CNT 7 THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS RECORD  
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 2 OF 6 CAPLUS COPYRIGHT 2003 ACS on STN  
AN 2002:116982 CAPLUS  
DN 137:47425  
TI Evolution, synthesis and SAR of tripeptide .alpha.-ketoacid inhibitors of the hepatitis C virus NS3/NS4A serine protease  
AU Colarusso, Stefania; Gerlach, Benjamin; Koch, Uwe; Muraglia, Ester; Conte, Immacolata; Stansfield, Ian; Matassa, Victor G.; Narjes, Frank  
CS Department of Chemistry, MRL Rome, IRBM, Rome, Pomezia, 00040, Italy  
SO Bioorganic & Medicinal Chemistry Letters (2002), 12(4), 705-708  
CODEN: BMCL8; ISSN: 0960-894X  
PB Elsevier Science Ltd.  
DT Journal  
LA English  
OS CASREACT 137:47425

RE.CNT 15 THERE ARE 15 CITED REFERENCES AVAILABLE FOR THIS RECORD  
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 3 OF 6 CAPLUS COPYRIGHT 2003 ACS on STN  
AN 2002:116981 CAPLUS  
DN 137:149812  
TI A designed P1 cysteine mimetic for covalent and non-covalent inhibitors of HCV NS3 protease  
AU Narjes, Frank; Koehler, Konrad F.; Koch, Uwe; Gerlach, Benjamin; Colarusso, Stefania; Steinkuhler, Christian; Brunetti, Mirko; Altamura, Sergio; De Francesco, Raffaele; Matassa, Victor G.  
CS Department of Chemistry, MRL Rome, IRBM, Rome, Pomezia, 00040, Italy  
SO Bioorganic & Medicinal Chemistry Letters (2002), 12(4), 701-704  
CODEN: BMCL8; ISSN: 0960-894X  
PB Elsevier Science Ltd.  
DT Journal  
LA English

RE.CNT 27 THERE ARE 27 CITED REFERENCES AVAILABLE FOR THIS RECORD  
ALL CITATIONS AVAILABLE IN THE RE FORMAT

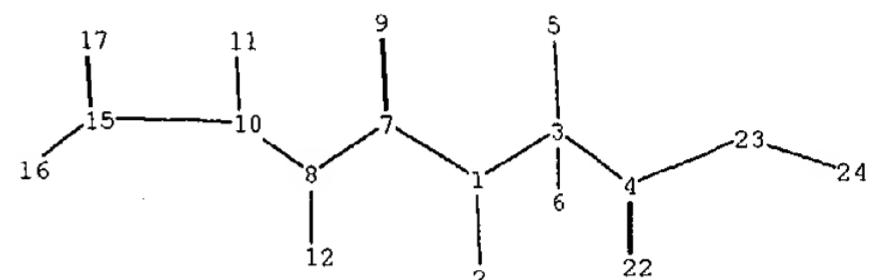
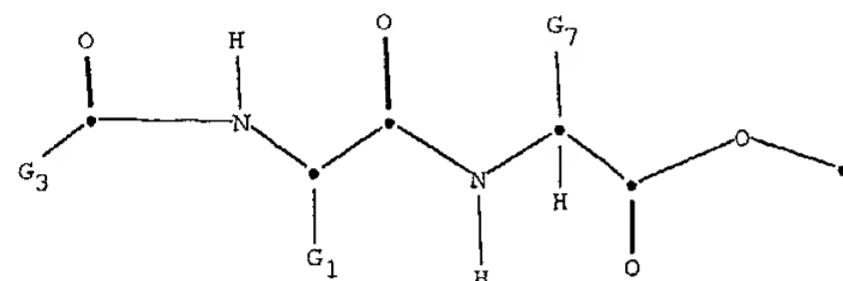
L3 ANSWER 4 OF 6 CAPLUS COPYRIGHT 2003 ACS on STN  
AN 2000:352482 CAPLUS  
DN 133:189820  
TI Probing the active site of the hepatitis C virus serine protease by fluorescence resonance energy transfer  
AU Fattori, Daniela; Urbani, Andrea; Brunetti, Mirko; Ingenito, Raffaele; Pessi, Antonello; Prendergast, Kristine; Narjes, Frank; Matassa, Victor G.; De Francesco, Raffaele; Steinkuhler, Christian  
CS Istituto di Ricerche di Biologia Molecolare "P. Angeletti", Rome, 00040, Italy  
SO Journal of Biological Chemistry (2000), 275(20), 15106-15113  
CODEN: JBCHA3; ISSN: 0021-9258  
PB American Society for Biochemistry and Molecular Biology  
DT Journal  
LA English

RE.CNT 42 THERE ARE 42 CITED REFERENCES AVAILABLE FOR THIS RECORD  
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 5 OF 6 CAPLUS COPYRIGHT 2003 ACS on STN  
AN 2000:68910 CAPLUS  
DN 132:245829  
TI .alpha.-Ketoacids Are Potent Slow Binding Inhibitors of the Hepatitis C Virus NS3 Protease  
AU Narjes, Frank; Brunetti, Mirko; Colarusso, Stefania; Gerlach, Benjamin; Koch, Uwe; Biasioli, Gabriella; Fattori, Daniela; De Francesco, Raffaele; Matassa, Victor G.; Steinkuehler, Christian  
CS Departments of Biochemistry Medicinal Chemistry and Computational Chemistry, Istituto di Ricerche di Biologia Molecolare (IRBM) P. Angeletti, Pomezia, 00040, Italy  
SO Biochemistry (2000), 39(7), 1849-1861  
CODEN: BICHAW; ISSN: 0006-2960  
PB American Chemical Society  
DT Journal  
LA English

RE.CNT 58 THERE ARE 58 CITED REFERENCES AVAILABLE FOR THIS RECORD  
ALL CITATIONS AVAILABLE IN THE RE FORMAT

C:\Program Files\Stnexp\Queries\fluorinesub.str



chain nodes :

1 2 3 4 5 6 7 8 9 10 11 12 15 16 17 22 23 24

chain bonds :

1-2 1-3 1-7 3-4 3-5 3-6 4-22 4-23 7-8 7-9 8-10 8-12 10-11 10-15 15-17  
15-16 23-24

exact/norm bonds :

1-3 1-7 3-5 4-22 4-23 7-9 8-10 8-12 10-15 15-17 15-16 23-24

exact bonds :

1-2 3-4 3-6 7-8 10-11

G1:Ak,CH3

G2:H,CF3,OH

G3:Cb,Ak

G4:C,N

G5:O,S,NH,N

G6:H,Cb,Ak

G7:CF2,CF3,F

Match level :

1:CLASS 2:CLASS 3:CLASS 4:CLASS 5:CLASS 6:CLASS 7:CLASS 8:CLASS 9:CLASS 10:CLASS  
11:CLASS 12:CLASS 15:CLASS 16:CLASS 17:CLASS 22:CLASS 23:CLASS 24:CLASS

L3 ANSWER 6 OF 6 CAPLUS COPYRIGHT 2003 ACS on STN  
AN 1999:795834 CAPLUS  
DN 132:36034  
TI Preparation of peptide inhibitors of hepatitis C virus NS3 protease  
IN Matassa, Victor; Narjes, Frank; Koehler, Konrad; Ontoria, Jesus; Poma, Marco; Marchetti, Antonella  
PA Istituto Di Ricerche Di Biologia Molecolare P Angeletti S.p.A., Italy  
SO PCT Int. Appl., 121 pp.  
CODEN: PIXXD2

DT Patent  
LA English

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 9964442	A1	19991216	WO 1999-GB1824	19990609
	W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
	RW: GH, GM, KE, LS, MW, SD, SL, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
	CA 2330247	AA	19991216	CA 1999-2330247	19990609
	AU 9942798	A1	19991230	AU 1999-42798	19990609
	AU 754773	B2	20021121		
	EP 1084137	A1	20010321	EP 1999-955475	19990609
PRAI	GB 1998-12523	A	19980610		
	WO 1999-GB1824	W	19990609		

RE.CNT 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD  
ALL CITATIONS AVAILABLE IN THE RE FORMAT

uploading fluorinesub.str

L1 STRUCTURE UPLOADED

=> l1 sss full  
FULL SEARCH INITIATED 09:54:20 FILE 'REGISTRY'  
FULL SCREEN SEARCH COMPLETED - 137400 TO ITERATE

100.0% PROCESSED 137400 ITERATIONS 33156 ANSWERS  
SEARCH TIME: 00.00.06

L2 33156 SEA SSS FUL L1

=> file caplus  
COST IN U.S. DOLLARS SINCE FILE TOTAL  
FULL ESTIMATED COST ENTRY SESSION  
148.15 148.36

FILE 'CAPLUS' ENTERED AT 09:54:38 ON 26 SEP 2003  
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.  
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.  
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FILE COVERS 1907 - 26 Sep 2003 VOL 139 ISS 14  
FILE LAST UPDATED: 25 Sep 2003 (20030925/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

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L3 8558 L2

=> 13 and py<2000  
19719654 PY<2000  
L4 7788 L3 AND PY<2000

=> 13 and py<1999  
18916701 PY<1999  
L5 7538 L3 AND PY<1999

=> d hitstr 1

L5 ANSWER 1 OF 7538 CAPLUS COPYRIGHT 2003 ACS on STN  
IT \*\*\*145643-18-1\*\*\* \*\*\*175071-81-5\*\*\*  
RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses)  
(topical gels contg. N-[5-[4-(aminoiminomethyl)phenyl]-1-oxopentyl]-  
1-.alpha.-aspartyl]-L-phenylalanines)  
RN 145643-18-1 CAPLUS  
CN L-Phenylalanine, N-[5-[4-(aminoiminomethyl)phenyl]-1-oxopentyl]-L-.alpha.-  
aspartyl-, dimethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

/ structure 1 in file .gra /

RN 175071-81-5 CAPLUS  
CN L-Phenylalanine, N-[5-[4-(aminoiminomethyl)phenyl]-1-oxopentyl]-L-.alpha.-  
aspartyl-, diethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

/ structure 2 in file .gra /

=> d hitstr 2

L5 ANSWER 2 OF 7538 CAPLUS COPYRIGHT 2003 ACS on STN  
IT \*\*\*149231-77-6\*\*\*  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(prepn. of chromophore-contg. peptides for use in detg.  
interleukin-1.beta. convertase activity)  
RN 149231-77-6 CAPLUS  
CN L-Alanine, N-acetyl-L-tyrosyl-L-valyl-, phenylmethyl ester (9CI) (CA  
INDEX NAME)

Absolute stereochemistry.

/ structure 3 in file .gra /

L1 STRUCTURE UPLOADED

=> l1 sss full  
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100.0% PROCESSED 144804 ITERATIONS 33156 ANSWERS  
SEARCH TIME: 00.00.05

L2 33156 SEA SSS FUL L1

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=> 12  
L3 8558 L2

=> 12 and py<1999  
8558 L2  
18916701 PY<1999

L4 7538 L2 AND PY<1999

=> 13 and py<1999  
18916701 PY<1999

L5 7538 L3 AND PY<1999

=> d hitstr 1

L5 ANSWER 1 OF 7538 CAPLUS COPYRIGHT 2003 ACS on STN  
IT \*\*\*145643-18-1\*\*\* \*\*\*175071-81-5\*\*\*

RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses)  
(topical gels contg. N-[N-[5-[4-(aminoiminomethyl)phenyl]-1-oxopentyl]-  
1-.alpha.-aspartyl]-L-phenylalanines)

RN 145643-18-1 CAPLUS

CN L-Phenylalanine, N-[5-[4-(aminoiminomethyl)phenyl]-1-oxopentyl]-L-.alpha.-  
aspartyl-, dimethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

/ Structure 4 in file .gra /

RN 175071-81-5 CAPLUS

CN L-Phenylalanine, N-[5-[4-(aminoiminomethyl)phenyl]-1-oxopentyl]-L-.alpha.-  
aspartyl-, diethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

/ Structure 5 in file .gra /

=>  
Uploading fluorinesub.str

L6 STRUCTURE UPLOADED

=> 16 sss full

FULL SEARCH INITIATED 10:04:28 FILE 'REGISTRY'  
FULL SCREEN SEARCH COMPLETED - 75 TO ITERATE

100.0% PROCESSED 75 ITERATIONS  
SEARCH TIME: 00.00.01

2 ANSWERS

L7 2 SEA SSS FUL L6

=> file caplus  
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FULL ESTIMATED COST

SINCE FILE ENTRY	TOTAL SESSION
148.15	303.74

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FILE COVERS 1907 - 26 Sep 2003 VOL 139 ISS 14  
FILE LAST UPDATED: 25 Sep 2003 (20030925/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> 17

L8 1 L7

=> d hitstr 1

L8 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2003 ACS on STN  
IT \*\*\*149075-80-9P\*\*\* \*\*\*149075-81-0P\*\*\*  
RL: SPN (Synthetic preparation); PREP (Preparation)  
(prepn. of)  
RN 149075-80-9 CAPLUS  
CN Alanine, 3,3,3-trifluoro-N-[N-[N-[(phenylmethoxy)carbonyl]-L-leucyl]-L-alanyl]-, methyl ester (9CI) (CA INDEX NAME)

/ Structure 6 in file .gra /

RN 149075-81-0 CAPLUS  
CN Alanine, 3,3,3-trifluoro-N-[N-[N-[(phenylmethoxy)carbonyl]glycyl]-L-phenylalanyl]-, methyl ester (9CI) (CA INDEX NAME)

/ Structure 7 in file .gra /

=> d bib 1

L8 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2003 ACS on STN  
AN 1993:496134 CAPLUS  
DN 119:96134  
TI Peptide modification by incorporation of .alpha.-trifluoromethyl .alpha.-amino acids via trifluoromethyl-substituted acylimines  
AU Hoess, E.; Rudolph, M.; Seymour, L.; Schierlinger, C.; Burger, K.  
CS Org.-Chem. Inst., Tech. Univ. Muenchen, Garching, W-8046, Germany  
SO Journal of Fluorine Chemistry (1993), 61(1-2), 163-70  
CODEN: JFLCAR; ISSN: 0022-1139  
DT Journal  
LA English  
OS CASREACT 119:96134

=> FIL STNGUIDE

COST IN U.S. DOLLARS

	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	4.80	308.54

FILE 'STNGUIDE' ENTERED AT 10:07:00 ON 26 SEP 2003  
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AND TECHNOLOGY CORPORATION, AND FACHINFORMATIONSZENTRUM KARLSRUHE

FILE CONTAINS CURRENT INFORMATION.  
LAST RELOADED: Sep 19, 2003 (20030919/UP).